# Enhanced graph-learning schemes driven by similar distributions of motifs

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- Graph-based methods are a popular option to process contemporary data
  - Graph topology useful to model underlying irregular structure
  - The graph topology is unknown in many relevant applications

Road network

Social network

Home automation network

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- Graph learning: estimates the graph topology from nodal observations
  - Properties of the signals depend on the topology

# Context and goal

- Graph learning is a well-studied problem with many different approaches
  - Assuming different relation between the graph and the data
  - Smoothness, Gaussianity, stationarity [Dong16][Friedman08][Segarra17]

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  - Smoothness, Gaussianity, stationarity [Dong16][Friedman08][Segarra17]
- **Limitation**: focus placed on the model relating graphs and signals
  - Prior graph structural information is rarely considered
- Works starting to pay attention to this problem
  - Joint network inference [Navarro24]
  - Spectral Laplacian constraints [Kumar19]
  - Graphon-based method [Roddenberry21]

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  - Joint network inference [Navarro24]
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  - Graphon-based method [Roddenberry21]
- **Contribution**: exploit motif density information when learning a graph
  - Assuming observed signals are Gaussian

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- Graph $G = (V, E)$ with $N$ nodes and adjacency $\mathbf{A}$
  - ⇒ $A_{ij}$ = Proximity between $i$ and $j$
- Define a signal $\mathbf{x} \in \mathbb{R}^N$ on top of the graph
  - ⇒ $x_i$ = Signal value at node $i$
- Associated with $G$ is the graph-shift operator $\mathbf{S} \in \mathbb{R}^{N \times N}$ (e.g. $\mathbf{A}$, $\mathbf{L}$)
  - ⇒ $S_{ij} \neq 0$ if $i = j$ or $(i, j) \in E$ (local structure in $G$)
  - ⇒ Diagonalized as $\mathbf{S} = \mathbf{V}\mathrm{diag}(\ )\mathbf{V}^{-1}$

# Notation and preliminaries

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- Graph $G = (V, E)$ with $N$ nodes and adjacency $\mathbf{A}$
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  - $\Rightarrow$ Diagonalized as $\mathbf{S} = \mathbf{V}\mathrm{diag}(\ )\mathbf{V}^{-1}$
- **Motifs** are subgraphs with a specific pattern (e.g., star graph, triangle)
  - $\Rightarrow$ Density of motifs measures the frequency with which a motif appears

# Motif density from a reference graph

- Knowing the true motifs distribution of $G$ is useful but unrealistic
- Assume access to a reference graph $\tilde{G}$ with a similar motif distribution
  - Learn $G$ with a similar distribution to that of $\tilde{G}$
  - Similar assumption to joint graph learning methods

# Motif density from a reference graph



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**Why density of motifs?**

- The density of motifs can be computed **locally**
  - Allows comparing graphs of different sizes
  - It can be approximated from a subgraph of $\tilde{G}$
- Requiring similar motifs is laxer assumption than similar support

**Problem statement**

- Let $\mathbf{S}$ be the GSO of the unknown graph $\mathcal{G}$
- Given $M$ graph signals $\mathbf{X} := [\mathbf{x}^{(1)}, ..., \mathbf{x}^{(M)}] \in \mathbb{R}^{N \times M}$
  - ⇒ Sampled from a Gaussian distribution $\mathbf{x}^{(m)} \sim \mathcal{N}(\mathbf{0}, \mathbf{S}^{-1})$
- Given a reference graph $\tilde{\mathcal{G}}$ with eigenvalues ~
  - ⇒ With a similar density of motifs to that of the sought graph
- **Goal**: find the maximum likelihood estimator $\hat{\mathbf{S}}$

# Graph learning driven by motifs

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**Challenges**

- How to tractably compare densities of motifs of two graphs?
- How to incorporate motif information into the MLE?
  - Optimization problem will most likely be non-convex

# From motif density to spectral test functions

- Computing the density of motifs of a graph is a combinatorial task
- Consider evaluating a test function $g(\ )$ over the spectral distribution

$$c_g(\ ) = \int g(\ )\, d\ (\ ) = \frac{1}{N} \sum_{i=1}^{N} g(\ _i)$$

  ) With empirical spectral density function

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**Theorem**

Let $G$ and $\tilde{G}$ be two graphs such that the distance between their densities of motifs is upper-bounded by . Then

$$|c_g(\ )\quad c_g(\tilde{\ })| \qquad + \ _r$$

- Similar densities of motifs render similar values when evaluating $c_g(\ )$
  - Enables easy integration into an optimization problem
  - Less expressive than motive densities in describing the structure

- We have a tractable approach to harnessing information about motif density
  - Evaluating a test function over the spectrum of S and S
- The constrained maximum likelihood estimator is given by

$$\min_{\mathbf{S};\mathbf{V};} \ \mathrm{tr}(\hat{\mathbf{C}}\mathbf{S}) \quad \log\det(\mathrm{diag}(\ \ )) + \quad \|\mathbf{S}\|_1 + \frac{}{2}\|\mathbf{S} \quad \mathbf{V}\mathrm{diag}(\ \ )\mathbf{V}^\top\|_F^2$$

$$\mathrm{s.t.}: \quad |c_g(\ \ ) \quad c_g(\tilde{\ })| \quad ; \ \mathbf{S} \in \mathcal{S}; \ \mathbf{V}^\top\mathbf{V} = \mathbf{I}.$$

  - Similarity constraint stems from similar motifs of $G$ and $\tilde{G}$
  - $c_g(\tilde{\ })$ is a constant obtained from $\tilde{\mathbf{S}}$
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  - Similarity constraint stems from similar motifs of $G$ and $\tilde{G}$
  - $c_g(\tilde{\ })$ is a constant obtained from $\tilde{\mathbf{S}}$
  - Spectrum of S is close to the one satisfying similarity constraint
- Solving the resulting non-convex optimization problem is non-trivial
  - Similarity constraint will be non-convex for most test functions
  - Orthogonality of V and bilinear terms involving V and and

- Focus on **concave test functions** $g$
- Split constraint into concave/convex terms avoiding function composition

$$|c_g( \quad ) \quad c_g(\tilde{\ })| \qquad = ) \quad c_g( \quad ) \quad c_g(\tilde{\ }) + \quad ; \quad c_g( \quad ) \quad c_g(\tilde{\ })$$

- Reformulate the optimization problem as

$$\min_{\mathbf{S};\mathbf{V};} \ \mathrm{tr}(\hat{\mathbf{C}}\mathbf{S}) \quad \log\det(\mathrm{diag}( \quad )) + \quad \|\mathbf{S}\|_1 \ + \frac{}{2}\|\mathbf{S} \quad \mathbf{V}\mathrm{diag}( \quad )\mathbf{V}^\top\|_F^2 + \quad c_g( \quad )$$

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  ⇒ Convex feasible set yet non-convex objective

# Relaxed similarity constraints

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- Reformulate the optimization problem as

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- Approximate concave term minimizing an upper bound as in MM

$$u(\;;\;^{(t-1)}) = \nabla c_g(\;^{(t-1)})^\top$$

- Iterative alternating minimization algorithm to avoid biconvexity
  - Similar to the approach introduced in [Kumar2019]

**Step 1**: Solved approximately in closed-form

$$\mathbf{S}^{(t+1)} = \operatorname*{argmin}_{\mathbf{S}\in\mathcal{S}} \mathrm{tr}(\hat{\mathbf{C}}\mathbf{S}) + \alpha\|\mathbf{S}\|_1 + \frac{\beta}{2}\|\mathbf{S} - \mathbf{V}^{(t)}\mathbf{\Lambda}^{(t)}\mathbf{V}^{(t)\top}\|_F^2$$

**Step 2**. Solution given by eigendecomposition of $\mathbf{S}^{(t+1)}$

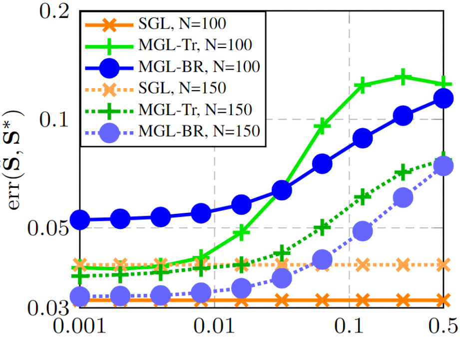
$$\mathbf{V}^{(t+1)} = \operatorname*{argmin}_{\mathbf{V}} \frac{\beta}{2}\|\mathbf{S}^{(t+1)} - \mathbf{V}\mathbf{\Lambda}^{(t)}\mathbf{V}^\top\|_F^2 \;\; \text{s.t}: \;\; \mathbf{V}^\top\mathbf{V} = \mathbf{I}$$

**Step 3**. Solved with over-the-shelf cvx solver

$$\boldsymbol{\lambda}^{(t+1)} = \operatorname{argmin} - \sum_{j=1}^{N} \log(\boldsymbol{\lambda}_j) + \frac{\beta}{2}\|\boldsymbol{\lambda} - \hat{\boldsymbol{\lambda}}\|_2^2 + \gamma u(\boldsymbol{\lambda}, \boldsymbol{\lambda}^{(t)}) \;\; \text{s.t}: \;\; c_g(\boldsymbol{\lambda}) \geq c_g(\tilde{\boldsymbol{\lambda}}) - \delta$$

- The algorithm is guaranteed to converge to a stationary point
- Computational complexity of $O(N^3)$

- Assess the influence of discrepancies between $G$ and $\tilde{G}$
  - $G$: SBM graph with 100/150 nodes and 5 disconnected communities
  - Setting tailored to GSL method



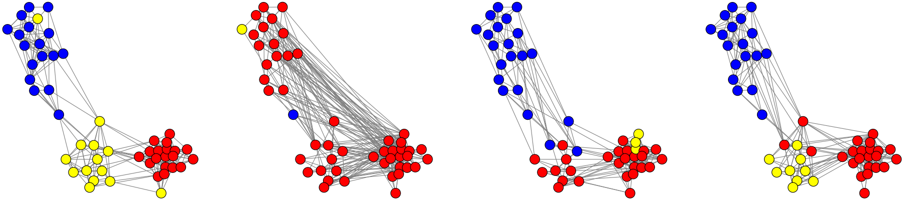

(c) Intercluster probability

- MGL robust to discrepancies in the intercluster connectivity
  - Information in $\tilde{G}$ beyond conn. comp.
- Error of MGL improves with $N$
  - $N = 150$ outperforms SGL
  - Similarity constraint more informative for large graphs

# Numerical evaluation - Real world data



- Dataset contains votes of the US Senate
  - Political graph is inferred from senators votes
  - $G$ is the 115th congress and $\tilde{G}$ is the 114th
  - Labels represent ideological representation (Rep, Dem, Mix)
- First we learn the graph topology using 100 observations
  - Then use spectral clustering to infer node labels



Ground truth — Unc. — SGL — MGL-BR

# Conclusions and future work

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- We proposed a tractable approach to leverage graph structural information
  - Assume access to a reference graph with a similar motif density
  - Evaluate a test function over the graph spectrum
  - Relation motif density/test function applicable to other tasks
- The density of motifs and the similarity constraint can be computed locally
  - Allows to compare graphs of different sizes
  - Is less restrictive than other assumptions
- The MLE with the similarity constraint was a non-convex problem
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**Future research direction**

- Exploit information about motifs as prior information in other GSP tasks
  - Settings with hidden variables or imperfect topology knowledge
- Characterize and design good test functions

# Questions?

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- Paper [Rey23] available at QR


Questions at: **samuel.rey.escudero@urjc.es**

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